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A parallel fast multipole method for elliptic difference equations

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ABSTRACT

A new fast multipole formulation for solving elliptic difference equations on unbounded domains and its parallel implementation are presented. These difference equations can arise directly in the description of physical systems, e.g. crystal structures, or indirectly through the discretization of PDEs. In the analog to solving continuous inhomogeneous differential equations using Green's functions, the proposed method uses the fundamental solution of the discrete operator on an infinite grid, or lattice Green's function. Fast solutions $\mathcal{O}(N)$ are achieved by using a kernel-independent interpolation-based fast multipole method. Unlike other fast multipole algorithms, our approach exploits the regularity of the underlying Cartesian grid and the efficiency of FFTs to reduce the computation time. Our parallel implementation allows communications and computations to be overlapped and requires minimal global synchronization. The accuracy, efficiency, and parallel performance of the method are demonstrated through numerical experiments on the discrete 3D Poisson equation.

1. Introduction

Numerical simulations of physical phenomena often require fast solutions to linear, elliptic difference equations with constant coefficients on regular, unbounded domains. These difference equations naturally arise in the description of physical phenomena including random walks [1], crystal physics [2], and quantum mechanics [3]. Additionally, such difference equations can result from the discretization of PDEs on infinite regular grids or meshes [4–7]. Apart from the accuracy with which the underlying PDE is solved, accurate solution of the difference equations themselves is relevant for compatible spatial discretization schemes that enforce discrete conservation laws [8,9]. Examples of these techniques include finite-volume methods, mimetic schemes, covolume methods, and discrete calculus methods.

The present method considers difference equations formally defined on unbounded Cartesian grids. Solutions to the difference equations are obtained through the convolution of the fundamental solution of the discrete operator with the source terms of the difference equations. As a result, the formally infinite grid can be truncated to a finite computational grid by removing cells that contain negligible source strength. The ease with which this technique is able to adapt the computational domain makes it well-suited for applications involving the temporal evolution of irregular source distributions. For problems that are efficiently described by block-structured grids it is possible adapt the computational domain by simply adding or removing blocks; an example of this technique applied to an incompressible flow is provided in Section 5.

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The fundamental solution of discrete operators on regular grids, or lattices, are often referred to as lattice Green's functions (LGFs). Expressions for LGFs can be readily obtained in the form of Fourier integrals, but it is typically not possible to reduce the integral representations to expressions only involving a few elementary functions [10,11]. The analytical treatment and the numerical evaluation of many LGFs is facilitated by the availability of asymptotic expansions [12–14]. Although LGFs have been extensively studied, they have rarely been used for solving large systems of elliptic difference equations (exceptions include 2D problems [15,6,7]). The present work extends the use of LGFs to large scale computations involving solutions to 3D elliptic difference equations.

Solving the system of difference equations using LGFs requires evaluating discrete convolutions of the form

$$u(\mathbf{x}_i) = [K * \mathbf{f}](\mathbf{x}_i) = \sum_{j=0}^{M-1} K(\mathbf{x}_i, \mathbf{y}_j) f(\mathbf{y}_j), \quad i = 0, 1, \ldots, N-1, \tag{1}$$

where $K(\mathbf{x}_i, \mathbf{y}_j)$ is the kernel describing the influence of a source located at $\mathbf{y}_j$ with strength $f(\mathbf{y}_j)$ has on the field $u(\mathbf{x})$ at location $\mathbf{x}_i$. For the case of $M = N$, the straightforward approach to evaluate Eq. (1) requires $\mathcal{O}(N^2)$ operations. There are several techniques for evaluating Eq. (1) in $\mathcal{O}(N)$ or $\mathcal{O}(N \log N)$ operations. A few of these techniques are FMMs, FFT-based methods, particle-in-cell methods, particle-mesh methods, multigrid techniques, multilevel local-correction methods, and hierarchical matrix techniques. In the interest of brevity, a literature review of all the methods related to the fast evaluation of Eq. (1) is omitted; instead we focus our attention on FMMs.

The performance of FMMs relies on the existence of a compressed, or low-rank, representation of the far-field behavior of $K(\mathbf{x}, \mathbf{y})$ that can be used to evaluate Eq. (1) to a prescribed tolerance. Classical fast multipole methods [16,17] require analytical expansions of the far-field behavior of kernels in order to derived low-rank approximations. Although classical FMMs can be developed for the asymptotic expansion of LGFs, alternative FMMs that are better suited for complicated kernel expressions have been developed. Kernel-independent FMMs [18–22,7] do not require analytical expansions of the far-field; instead, for suitable kernels, these methods only require numerical evaluations of the kernel.

The present method is a kernel-independent interpolation-based FMM for non-oscillatory translation-invariant kernels [23,21]. These FMMs achieve low-rank approximations of the kernel by projecting the kernel onto a finite basis of interpolation functions. Interpolation-based FMMs [23,21] use Chebyshev interpolation and accelerate convolutions involving the compressed kernel using singular-value-decompositions (SVDs). In contrast, our method uses polynomial interpolation on equidistant nodes and accelerates convolutions involving the compressed kernel using FFTs. The use of intermediate regular grids and fast FFT-based convolutions have been used by other FMMs [24,25,19,26], and shown to particularly useful in accelerating the computations of 3D methods [19]. The use of intermediate regular grids in our method has the added advantage of simplifying the multilevel algorithm, since sources and evaluation points are defined on Cartesian grids at all levels of the multilevel scheme. The spatial regularity allows for the same fast convolution techniques to be used in determining near-field and far-field contributions. In addition to the base algorithm, our method allows for pre-computations that further accelerate the solver.

The present FMM is similar to the recent 2D FMM [7] in that they both solve difference equations on unbounded domains. In contrast to our method, this method uses skeleton/proxy points and rank-revealing factorizations to obtain low-rank approximations of the kernel. Although we think it is possible to extend this method to 3D, we refrain from speculating on the performance of the algorithm since such extensions are not explored in current literature and their details are unclear to us.

Details regarding LGFs and their relation to solving difference equations on unbounded domains are presented in Section 2. This section also describes methods for performing fast convolutions based on kernel compression and FFT techniques, and presents a context in which these two techniques can combined to yield an even faster convolution scheme. The resulting fast multipole algorithm and its parallel extension are then described in Section 3. Finally, serial and parallel numerical experiments are reported and analyzed in Section 4.

2. Lattice Green's functions and fast block-wise convolution techniques

2.1. Solving difference equations on infinite Cartesian grids

The method proposed in this paper is designed to solve inhomogeneous, linear, constant-coefficient difference equations on unbounded domains. As a representative problem, we consider in detail the difference equations resulting from the discretization of Poisson's equation in 3D. Consider the Poisson equation

$$[\Delta u](\mathbf{x}) = f(\mathbf{x}), \quad supp(f) \in \Omega, \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^3$, Ω is a bounded domain in $\mathbb{R}^3$, and $u(\mathbf{x})$ decays as $1/|\mathbf{x}|$ at infinity. Eq. (2) has the analytic solution

$$u(\mathbf{x}) = [G * f](\mathbf{x}) = \int_{\Omega} G(\mathbf{x} - \boldsymbol{\xi}) f(\boldsymbol{\xi})\, d\boldsymbol{\xi}, \tag{3}$$

where $G(\mathbf{x}) = -1/4\pi|\mathbf{x}|$ is the fundamental solution of the Laplace operator. Discretizing Eq. (2) on an infinite uniform Cartesian grid using a standard second-order finite-difference or finite-volume scheme produces a set of difference equations